

Need for calculation of coupled wave functions

Coupled channel bound states calculations for alkali dimers using the Fourier grid method

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$$\mathbf{H}\psi = (\mathbf{T} + \mathbf{V})\psi = E\psi.$$

$$V_{ij} = V(R_i) \delta_{ij}.$$

$$T_{ii} = \frac{\hbar^2}{4\mu L^2} \frac{N^2 + 2}{6},$$

$$T_{ij} = (-1)^{i-j} \frac{\hbar^2}{4\mu L^2} \frac{1}{\sin^2[(i-j)\pi/N]} \quad \text{for } i \neq j.$$

$$\begin{pmatrix} H_{AA} & H_{AB} \\ H_{BA} & H_{BB} \end{pmatrix} = \begin{pmatrix} \mathbf{T} & 0 \\ 0 & \mathbf{T} \end{pmatrix} + \begin{pmatrix} V_A & V_{AB} \\ V_{AB} & V_B \end{pmatrix},$$

+ Variable step size

